



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 12:40 PM EST

PDB ID : 5N23  
Title : Protein kinase A mutants as surrogate model for Aurora B with AT9283 inhibitor  
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Deposited on : 2017-02-07  
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

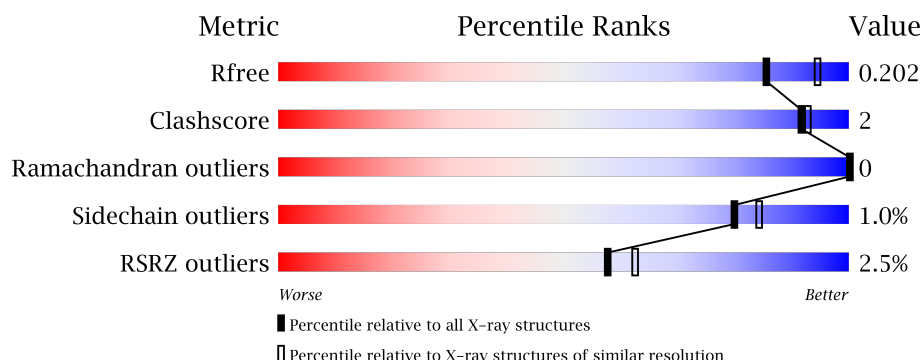
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4955 (2.10-2.06)
Clashscore	112137	5537 (2.10-2.06)
Ramachandran outliers	110173	5483 (2.10-2.06)
Sidechain outliers	110143	5484 (2.10-2.06)
RSRZ outliers	101464	4991 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
2	B	20	<div> <div>5%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3131 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	P	S	0	0	0
			2785	1798	466	510	4	7			

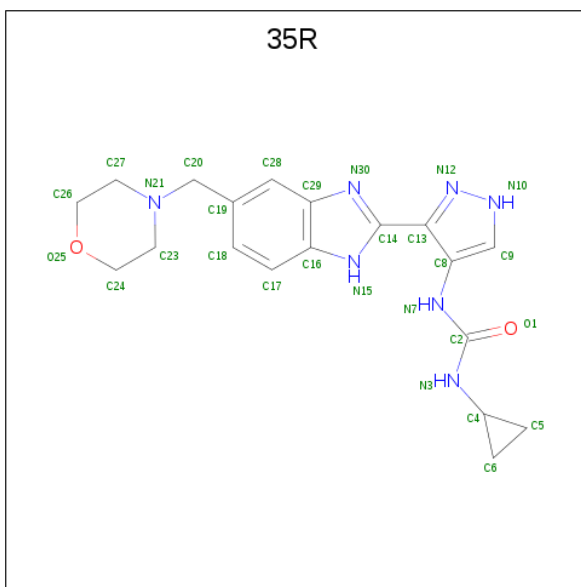
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ARG	LYS	engineered mutation	UNP P17612
A	95	GLN	LEU	engineered mutation	UNP P17612
A	120	LEU	MET	engineered mutation	UNP P17612
A	123	ALA	VAL	engineered mutation	UNP P17612
A	181	LYS	GLN	engineered mutation	UNP P17612
A	183	ALA	THR	engineered mutation	UNP P17612
A	195A	PRO	-	insertion	UNP P17612

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is 1-cyclopropyl-3-{3-[5-(morpholin-4-ylmethyl)-1H-benzimidazol-2-yl]-1H-pyrazol-4-yl}urea (three-letter code: 35R) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			56	38	14	4		

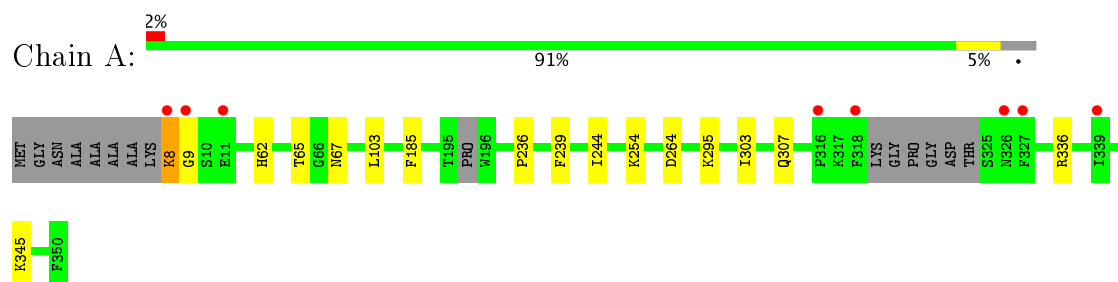
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	14	Total	O	0	0
			14	14		

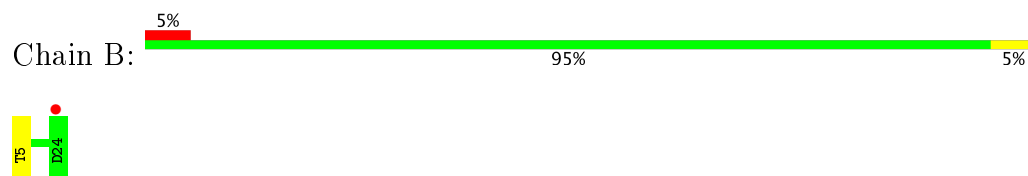
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.00Å 74.54Å 79.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.09 43.46 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.97-2.09) 97.3 (43.46-2.09)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.188 , 0.239 0.186 , 0.202	Depositor DCC
$R_{free}$ test set	1192 reflections (4.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 35R, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/2811	0.54	0/3782
2	B	0.44	0/159	0.54	0/212
All	All	0.41	0/2970	0.54	0/3994

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2735	11	1
2	B	157	0	146	0	1
3	A	56	0	46	0	0
4	A	119	0	0	0	0
4	B	14	0	0	0	0
All	All	3131	0	2927	11	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HG23	1:A:67:ASN:H	1.44	0.82
1:A:8:LYS:HE2	1:A:8:LYS:HA	1.67	0.76
1:A:244:ILE:H	1:A:244:ILE:HD12	1.54	0.69
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.62	0.63
1:A:303:ILE:O	1:A:307:GLN:HG2	2.08	0.54
1:A:8:LYS:HB3	1:A:9:GLY:HA3	1.89	0.53
1:A:236:PRO:HG2	1:A:239:PHE:HB3	1.96	0.48
1:A:62:HIS:HB3	1:A:65:THR:HG22	1.97	0.45
1:A:264:ASP:OD1	1:A:295:LYS:HE3	2.18	0.43
1:A:62:HIS:ND1	1:A:65:THR:HG22	2.34	0.42
1:A:254:LYS:HB2	1:A:254:LYS:HE3	1.91	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:NZ	2:B:5:THR:N[4_445]	1.74	0.46

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/352 (94%)	319 (97%)	10 (3%)	0	100	100
2	B	18/20 (90%)	18 (100%)	0	0	100	100
All	All	347/372 (93%)	337 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar



resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/301 (96%)	287 (99%)	3 (1%)	80	84
2	B	15/15 (100%)	15 (100%)	0	100	100
All	All	305/316 (96%)	302 (99%)	3 (1%)	80	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	336	ARG
1	A	345	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	10	1	9,9,10	1.65	1 (11%)	9,12,14	1.63	2 (22%)
1	SEP	A	139	1	9,9,10	1.62	2 (22%)	9,12,14	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	197	1	9,10,11	1.51	1 (11%)	10,14,16	1.02	0
1	SEP	A	338	1	9,9,10	1.54	2 (22%)	9,12,14	1.53	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	10	1	-	0/5/8/10	0/0/0/0
1	SEP	A	139	1	-	0/5/8/10	0/0/0/0
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/5/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	SEP	CA-C	2.48	1.53	1.50
1	A	338	SEP	CA-C	2.54	1.53	1.50
1	A	338	SEP	P-O1P	3.01	1.61	1.50
1	A	139	SEP	P-O1P	3.07	1.61	1.50
1	A	197	TPO	CA-C	3.18	1.54	1.50
1	A	10	SEP	P-O1P	3.71	1.63	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	SEP	P-OG-CB	-2.72	110.81	118.30
1	A	338	SEP	O2P-P-OG	2.03	112.14	106.73
1	A	10	SEP	OG-CB-CA	3.33	111.45	108.17
1	A	338	SEP	OG-CB-CA	3.48	111.60	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	35R	A	401[A]	-	31,32,32	2.69	11 (35%)	27,45,45	1.16	3 (11%)
3	35R	A	401[B]	-	31,32,32	2.76	12 (38%)	27,45,45	1.32	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	35R	A	401[A]	-	-	0/10/26/26	0/4/5/5
3	35R	A	401[B]	-	-	0/10/26/26	0/4/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401[B]	35R	C20-N21	-10.22	1.28	1.47
3	A	401[A]	35R	C20-N21	-10.21	1.28	1.47
3	A	401[A]	35R	C27-N21	-3.03	1.38	1.47
3	A	401[B]	35R	C27-N21	-2.98	1.38	1.47
3	A	401[A]	35R	C23-N21	-2.90	1.39	1.47
3	A	401[B]	35R	C23-N21	-2.88	1.39	1.47
3	A	401[A]	35R	C14-N15	-2.14	1.33	1.35
3	A	401[B]	35R	O1-C2	-2.02	1.19	1.23
3	A	401[B]	35R	C6-C4	2.08	1.53	1.48
3	A	401[A]	35R	C6-C4	2.11	1.53	1.48
3	A	401[A]	35R	C5-C4	2.16	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401[B]	35R	C5-C4	2.22	1.53	1.48
3	A	401[A]	35R	C13-C14	2.29	1.53	1.49
3	A	401[A]	35R	C20-C19	2.36	1.55	1.51
3	A	401[B]	35R	C13-C14	2.38	1.53	1.49
3	A	401[B]	35R	C9-C8	2.38	1.41	1.37
3	A	401[B]	35R	C20-C19	2.38	1.55	1.51
3	A	401[A]	35R	C8-N7	2.42	1.46	1.41
3	A	401[B]	35R	C8-N7	2.88	1.47	1.41
3	A	401[A]	35R	C2-N7	3.95	1.45	1.37
3	A	401[B]	35R	C2-N7	4.54	1.47	1.37
3	A	401[A]	35R	C2-N3	4.76	1.46	1.35
3	A	401[B]	35R	C2-N3	5.04	1.47	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401[A]	35R	C6-C4-N3	-3.22	113.97	118.66
3	A	401[B]	35R	O1-C2-N7	-2.07	120.05	123.58
3	A	401[A]	35R	C24-C23-N21	2.01	112.93	110.11
3	A	401[A]	35R	N7-C2-N3	2.43	117.70	113.84
3	A	401[B]	35R	N7-C2-N3	4.17	120.49	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	333/352 (94%)	-0.12	8 (2%) 59 63	24, 37, 63, 98	0
2	B	20/20 (100%)	0.33	1 (5%) 30 34	27, 31, 73, 78	0
All	All	353/372 (94%)	-0.09	9 (2%) 58 62	24, 36, 63, 98	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	12.4
1	A	8	LYS	6.3
1	A	9	GLY	5.5
1	A	326	ASN	4.1
1	A	327	PHE	3.2
1	A	316	PRO	2.6
2	B	24	ASP	2.5
1	A	11	GLU	2.4
1	A	339	ILE	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	10	10/11	0.73	0.24	-	43,77,88,94	0
1	SEP	A	338	10/11	0.97	0.10	-	37,47,58,60	0
1	SEP	A	139	10/11	0.92	0.14	-	35,46,71,71	0
1	TPO	A	197	11/12	0.99	0.13	-	24,27,29,32	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	35R	A	401[B]	28/28	0.89	0.17	0.80	28,34,59,64	28
3	35R	A	401[A]	28/28	0.89	0.17	0.72	28,33,59,64	28

### 6.5 Other polymers [i](#)

There are no such residues in this entry.